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I. INTRODUCTION

Besides its intrinsic interest in the theory of atomic collision, the detachment of electrons from $H^{(-)}$ by $e^{(-)}$ impact is of importance in certain branches of astrophysics. Consequently it has been studied both experimentally and theoretically by several authors in the past. In spite of this a number of divergencies prevail both among the theoretical calculations and the experimental observations. Experiments are done independently by Dance et al.[1] and by Tisone and Branscomb[2] and very recently, after this calculation has been completed, by Peart et al.[3] A discrepancy is seen to exist between the measurements of the first two groups, at higher energies (where the errors are expected to be smaller). Comparison of the measurements of Tisone and Branscomb with that of the last group[3] shows very close agreement over a large energy range provided a small adjustment due to normalisation of the two measurements at 100 e.v. is permitted. At around 10 e.v. (the region of lowest energy in all the measurements) the last two measurements differ significantly from that of the first group[1].

Theoretical calculations are done by several authors[4,5,6,7] over the past ten years and the results in general differ widely among each other. Moreover, apart from the works of Mcdowell and Williamson[5] and Bely and Schwartz[7] these calculations are widely different from all the experiments. The calculation of Mcdowell and Williamson[5], however, assumes plane wave approximation for the incident electron and applies an ad hoc correction for the coulomb effect, first introduced by Geltman[4], which brings their result relatively closer to the experiments above 20 e.v. At lower energies their theoretical approximations

have little justifications and the departure from the experiments is large (with or without the ad hoc coulomb correction). The calculation of Bely and Schwartz[7], on the other hand, uses the correct coulomb waves for the colliding electron but are obliged to use partial wave analysis. This, according to the authors, limits their numerical calculations to up to 60 e.v., above which too many partial waves, to be treated numerically, become important. In their investigations Bely and Schwartz use four different approximations for the ejected electron's wave function and conclude that the partial waves should be properly orthogonalised in order to obtain reasonable agreement with measurements.

In the present paper we have adopted an impact parameter method (much used in nuclear physics in connection with coulomb excitations of nuclei[8] and, in atomic physics, for excitation of neutral atoms[9], which overcomes the difficulty of adding contributions from numerous partial waves by an integration over the impact parameters. And the dominant coulomb repulsion of the incoming electron by the negatively charged ion is incorporated systematically by describing the motion of the colliding electron by a repulsive hyperbolic trajectory. The validity of such a replacement of Coulomb waves propagating at low energies by a Rutherford trajectory depends on the peculiar property of the coulomb field. It is well known that in scattering by a coulomb field the classical description depends on the largeness of the so-called Sommerfeld parameter η which is defined as $\eta = \frac{z_1 z_2}{v_1}$ where v_1 is the incident velocity and z_1 and z_2 are the effective charges on the ion and the electron respectively. Thus it is easily seen that the smaller the velocity of incidence the greater is η. For any inelastic process, such as the present one, a second condition need also to be satisfied in order that the trajectory description should be valid. The condition required

is that the difference between the initial and the final velocities should be small compared to the initial velocity itself. In our case the binding energy of $H^{(-)}$ being small the incident velocity could be lowered considerably witnout violating the condition. Nevertheless, in the end we shall apply a symmetrizing procedure to account for the change in velocity, by invoking the principle of detail balance.

II. MATHEMATICAL FORMULATION

We shall briefly sketch the mathematical formulation of electron detachment problem, closely paralleling the method of coulomb excitation in nuclear physics[8]. We shall use atomic units throughout this paper.

According to the time dependent scattering theory of Dirac[10] the transition amplitude between a state $|i>$ and a state $|f>$ is given by

$$T_{if} = -i \int_{-\infty}^{\infty} dt\, e^{i \Delta E_{if} t} \langle f | V_{eff.}(t) | i \rangle \qquad (1)$$

where $\Delta E_{if} = E_i - E_f$ is the difference of the initial and final energies and $V_{eff.}(t)$ is the effective interaction. For the present problem

$$V_{eff.}(t) = -\frac{1}{r(t)} + \frac{1}{|\vec{r}(t) - \vec{r}_1|} + \frac{1}{|\vec{r}(t) - \vec{r}_2|} - \frac{1}{r(t)} \qquad (2)$$

where $\vec{r}(t)$ is the position vector of the incident electron and $\vec{r}_1$ and $\vec{r}_2$ are the coordinates of the two target electrons, all measured from the nucleus (see Figure 1). We note that a term $\frac{1}{r(t)}$ of the total Hamiltonian of the system is utilised in obtaining the coulomb trajectory and hence is subtracted in the effective interaction (2). In the present calculation we have chosen to represent

the initial state of the $H^{(-)}$ by a variational wave function involving 20-correlated Hyllarus type terms:

$$\psi_i(\bar{r}_1, \bar{r}_2) = \frac{1}{\sqrt{2}}\left[e^{-\gamma r_1 - \delta r_2} \sum_{\ell mn} C_{\ell mn}\, r_1^{\ell} r_2^{m} r_{12}^{n} + 1 \longleftrightarrow 2\right] \tag{3}$$

This produces for the electron affinity $w_0 = -0.052772$ (a.u.) which compares with the 444-term calculation of Pekeris: $w_0 = -0.052775$ (a.u.). The reason for this choice is to leave no uncertainty in the target wave function so that the entire burden of approximation is borne by the rest of the theory. We approximate the final target state by a residual hydrogen atom and an outgoing free plane wave for the ejected electron:

$$\psi_f(\bar{r}_1, \bar{r}_2) = \frac{1}{\sqrt{2}}\left\{\phi_0(\vec{r}_1)\, e^{i\bar{k}\cdot\bar{r}_2} + \phi_0(\vec{r}_2)\, e^{i\bar{k}\cdot\bar{r}_1}\right\} \tag{4}$$

We now make the most vulnerable of our approximations by replacing the interaction (2) by its expansion in the outer region $r(t) > r_1, r_2$. We have

$$V_{eff.}(t) = \sum_{\lambda=1}^{\infty}\left\{\frac{r_1^{\lambda} P_\lambda\left(\hat{r}_1 \cdot \hat{r}(t)\right)}{r^{\lambda+1}(t)} + \frac{r_2^{\lambda} P_\lambda\left(\hat{r}_2 \cdot \hat{r}(t)\right)}{r^{\lambda+1}(t)}\right\} \tag{5}$$

where P_λ's are Legendre polynomials of order λ. In this approximation the transition integrals (I) can be factored out into matrix elements between the target states and a time integral over the projectile trajectory. We get

$$T_{if} = -i \sum \langle f \mid r_1^{\lambda} Y^*_{\lambda\mu}(\hat{r}_1) + r_2^{\lambda} Y^*_{\lambda\mu}(\hat{r}_2) \mid i \rangle \cdot J_{\lambda\mu} \tag{6}$$

where

$$J_{\lambda\mu} = \int_{-\infty}^{\infty} e^{i\Delta E_{if} t} \cdot \frac{Y_{\lambda\mu}\left(\hat{r}(t)\right)}{r^{\lambda+1}(t)} \, dt \, . \tag{7}$$

The orbit integrals $J_{\lambda\mu}$ are exactly the same as appear in the case of coulomb excitation of nuclei and are extensively studied in the literature[8]. We shall merely quote the results[8]

$$J_{\lambda\mu} = Y_\lambda^\mu\left(\frac{\pi}{2}, 0\right) \cdot \frac{1}{v_i a^\lambda} \cdot I_{\lambda\mu}(\xi, \theta) \tag{8}$$

where the constants

$$Y_\lambda^\mu\left(\frac{\pi}{2}, 0\right) = \left(\frac{2\lambda+1}{4\pi}\right)^{\frac{1}{2}} \frac{\{(\lambda-\mu)\,!\,(\lambda+\mu)\,!\}^{\frac{1}{2}}}{(\lambda+\mu)\,!!\,(\lambda-\mu)\,!!} (-1)^{\frac{\lambda+\mu}{2}}, \ \lambda+\mu \text{ even}. \tag{8a}$$

$$= 0, \ \lambda+\mu \text{ odd}.$$

$$a = \frac{z_1 z_2}{m_0 v_i^2} \tag{9}$$

$$\xi = \frac{a\,\Delta E_{if}}{v_i} \tag{10}$$

In the above v_i is the initial velocity, m_0 is the reduced mass and z_1 and z_2 are the effective charges on the target and the projectile, respectively.

Using the wave-functions (3) and (4) and performing all angular momentum algebra the target matrix element can be written as

$$\langle \psi_f(\vec{r}_1, \vec{r}_2) \,|\, r_1^\lambda Y_\lambda^{*}\mu(\hat{r}_1) + r_2^\lambda Y_\lambda^\mu(\hat{r}_2) \,|\, \psi_i(\vec{r}_1, \vec{r}_2) \rangle = B_\lambda(k) Y_\lambda^{*}\mu(\hat{k}) \tag{11}$$

where $B_\lambda(k)$ is a function of the wave number k of the ejected electron only.

The transition amplitude can now be written as

$$T_{if} = -i \sum \left(\frac{4\pi}{2\lambda + 1}\right) \cdot a^{-\lambda} v_i^{-1} Y_\lambda^\mu \left(\frac{\pi}{2}, 0\right) I_{\lambda\mu}(\xi, \theta) B_\lambda(k) Y_\lambda^{*}\mu(\hat{k}) \quad (12)$$

Defining the ejection angle integrated transition probability by

$$P_{if}(k|E_i) = \int |T_{if}|^2 \, d\hat{k}$$

and noting that the differential cross-section

$$d\sigma(k|E_i) = P_{if}(k|E_i) \cdot |2\pi b \, db|$$

where $b = a \cot \theta/2$ is the impact parameter and θ = angle of scattering we find

$$d\sigma(k|E_i) = \sum_{\lambda=1}^{\infty} (2\lambda + 1) |B_\lambda(k)|^2 a^{-2\lambda+2} v_i^{-2} \cdot df_\lambda(\xi, \theta) \quad (13)$$

and the total cross-section

$$\sigma(k|E_i) = \sum_{\lambda=1}^{\infty} (2\lambda + 1) |B_\lambda(k)|^2 a^{-2\lambda+2} v_i^{-2} f_\lambda(\xi) \quad (14)$$

where

$$df_\lambda(\xi, \theta) = \frac{4\pi^2}{(2\lambda + 1)^3} \sum_\mu |Y_\lambda\mu\left(\frac{\pi}{2}, 0\right) I_{\lambda\mu}(\xi, \theta)|^2 \frac{1}{\sin^4 \theta/2} \, d\Omega \quad (15)$$

and

$$f_\lambda(\xi) = \int \frac{d f_\lambda(\xi,\theta)}{d\Omega}\, d\Omega$$

$$= \frac{32\pi^3}{(2\lambda+1)^3} \sum_\mu \left| Y_{\lambda\mu}\left(\frac{\pi}{2}, 0\right)\right|^2 \int_1^\infty |I_{\lambda\mu}(\xi,\epsilon)|^2 \times \epsilon\, d\epsilon \qquad (16)$$

where ϵ is related to the scattering angle and hence the impact parameter by the relation $\epsilon = \sqrt{1 + (b/a)^2}$.

The results (13) and (14) do not take into account the change in the projectile velocity before and after the collision. This may be incorporated by symmetrizing the cross-sectional expressions with respect to the initial and final velocities as required by the principle of detail balance. This is most readily achieved by replacing Equations (9) and (10) by the following symmetrized expressions:

$$a \Rightarrow \frac{z_1 z_2}{m_0 v_i v_f}$$

$$\xi \Rightarrow z_1 z_2 \left(\frac{1}{v_f} - \frac{1}{v_i}\right)$$

and substituting them in Equations (13) and (14). To obtain the total cross-section of electron detachment for a given initial velocity and all ejection energies we must integrate over the energy of the ejected electron. Thus,

$$\sigma_{tot}(E_i) = \int_0^{k_{max}} dk\, k^2\, \sigma(k|E_i) \qquad (17)$$

where $k_{max.}$ is the maximum available momentum of ejection k, for a given energy of incidence E_i. In using (14) in (17) we are making a non-exchange approximation of the exact $\sigma(k|E_i)$ by the semiclassical expression (14), which does not include any exchange probability. In the event the probability of exchange is small the approximation should be good. For numerical calculations we have only to retain the leading term $\lambda = 1$ which corresponds to a dipole approximation of the interaction. Thus we need to evaluate the quantity $f_1(\xi)$ from Equation (16). Although $f_1(\xi)$ remains finite when integrated over all scattering angles (i.e., over all impact parameters), the multipole expansion of the potential necessitates a finite cut off at some non-zero minimum impact parameter b_0 (to eliminate unreliable contribution from the inner region) of the order of the radius of the detaching electron[9]. We therefore redefine the quantity $f_1(\xi)$ by the modified expression

$$\tilde{f}_1(\xi) = \frac{32\pi^3}{27} \sum_{\mu} \left| Y_{1\mu}\left(\frac{\pi}{2}, 0\right) \right|^2 \int_{\epsilon_0}^{\infty} |I_{1r}(\xi, \theta)|^2 \times \epsilon \, d\epsilon \qquad (18)$$

where

$$\epsilon_0 = \sqrt{\left(1 + \frac{b_0}{a}\right)^2}$$

We can perform the above integral over ϵ, analytically, and obtain

$$\tilde{f}_1(\xi) = -\frac{32\pi^2}{9} e^{-\pi\xi} (\xi\epsilon_0) K_{i\xi}(\xi\epsilon_0) K'_{i\xi}(\xi\epsilon_0) \qquad (19)$$

We note that for $b_0 = 0$, $\tilde{f}_1(\xi)$ coincides with the usual result quoted in Ref. (8).

For our present purpose we make the simplest choice of $b_0 = r_0$ where r_0 is the root mean square radius of the target, which we find to be 3.42 a_0, using our present wave function (3).

For comparison purposes we have also calculated the cross-section with another independent choice of

$$b_0 = \frac{1}{\sqrt{\Delta E_{if}}}$$

which estimates certain 'radial spread' of the detaching electron (ΔE_{if} being a measure of 'tightness of binding' of the detaching electron). It is clear from Table I that this choice of 'cut off' parameter yields essentially the same results as those from our first choice (which is simpler) for almost the entire energy range.

III. RESULTS AND DISCUSSIONS

Within the approximations introduced in this paper we have calculated the primary detachment cross-sections for the following two processes.

(i) $e^- + H^- \Rightarrow H(1S) + 2e^-$

(ii) $e^- + H^- \Rightarrow H(2S) + 2e^-$

In Table I we present results for process (i) with two different choices for the 'cut off' parameter.

In Figure 2 we compare our result (with $b_0 = r_0$) with the experiments of References 1, 2 and 3.

In Table II we present the results (with $b_0 = r_0$) for reaction (ii). Considering the smallness of this result compared to those in Table I we believe that almost the entire cross-section for electron detachment of H^- by collision with electron leaves residual hydrogen atom in its ground state.

Finally in Figure 3 we show typical energy distributions of ejected electrons for a few given incident energies.

We have noted that a change in the upper limit (as is sometimes done[5]) in Equation (17) from k_{max} to $k_{max}/2$ did not change our numerical results for the energy range considered.

Investigating the range of impact parameters further we found that when one integrates the Equation (18) for all impact parameters from 0 to ∞ one obtains cross-sections approximately twice as large as with our present cut off. If however, one normalises these data at a high energy with that obtained from Born approximation one obtains very close agreement for all energies (including the position of the peak) with the experiments of References 2 and 3.

Finally, we may qualitatively understand the applicability of the semiclassical model for the present calculation and its rather close agreement with experiments on the following grounds.

In single 'ionization' processes, such as the present detachment process, truly exchange phenomenon does not arise. It arises genuinely in the case of double ionization when the incident particle may be captured by the target and the two bound electrons may be ejected. This process being clearly of the second order is likely to contribute little for the single detachment cross-section.

The effect of 'exchange' in the single ionization case reduces to the classically analogous phenomenon of 'interference' (between the incident and the ejected electrons). However, in view of the calculated velocity distributions we find that the ejected electrons tend to concentrate at very low energy of ejection; this implies that the amount of interference is likely to be small except at the very lowest energies. At low energies, however, the incident electron is likely to be repelled away from the target electron, reducing the overlap and hence the exchange probability between the incident and the target electron. The same remark may be made for the validity of the outer expansion of the effective interaction at low energies and in the initial state. In the final state also the scattered electron may be found mostly to the outside of the ejected electron as indicated by the velocity distributions. At very high energies too, this situation being true, the penetration of the incident electron inside the target is unlikely to affect the outer expansion approximation drastically. This indicates that most of the contribution to the cross-section arises from 'outside' the target and hence a 'radial cut off' effectively eliminates the 'inner region' where the multipole expansion breaks down, without significantly affecting the total cross-section at the same time.

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